FY 2004 Major Initiative Areas

Advanced Nuclear Fuel Cycle Technology (Initiative leader: Phillip Finck, ERA)
If nuclear energy is to contribute to the energy supply in the future, it is necessary that we develop an improved nuclear system that addresses the waste and non-proliferation issues that both the U.S. and other countries will face this century. The essential components of such a system are a closed, proliferation resistant fuel cycle technology that can separate the long-lived actinides from spent fuel, and a fast spectrum reactor that can efficiently destroy these actinides by fission. The system must have a high degree of passive safety, and it must be economically competitive. The capability to provide multiple energy products is highly desirable. LDRD proposals that address innovative solutions to the technical and systems related issues of advanced fuel cycle technologies are invited. Subjects of interest include, but are not limited to, innovative reactor and fuel cycle concepts and systems studies, fuel cycle processes, supporting basic and engineering technology, and non-proliferation systems and technology.

Nanoscience (Initiative leader: Sam Bader, MSD & CNM)
This initiative seeks novel proposals that encompass the fabrication and characterization of nanoscale materials. Fabrication methods should highlight self-assembly and/or lithographic patterning; and nano-characterizations should embrace scanning probes or synchrotron X-ray nanoprobe techniques. The major scientific themes include: the exploration of the interface between the inorganic and the biomolecular realm, as well as bio-templating methods of nanofabrication, the exploration of carbon and/or complex oxide nanostructures, nanomagnetism and spintronics, and nanophotonics. Experimental and computational proposals are welcome. Computational ideas to investigate the rules that govern self-organization are especially sought.

Petaflops Computing and Computational Science (Initiative leader: Rick Stevens, MCS)
Argonne proposes a Petaflops Computing and Computational Science Initiative designed to make petaflops-scale computing systems a reality and to ensure that such systems are well suited to important scientific applications. Central to this initiative is the development and deployment of a petascale experimental research facility targeted at critical science and technology problems. Creation of such a facility will require dramatic extensions in computer hardware. Argonne researchers will explore new technologies, such as cluster-on-a-chip, to enable computers to scale to systems capable of trillions of operations per second. The primary targets for the petascale facility are the biosciences and nanosciences. Research is focusing on the development of a simulation system for modeling whole cells (initially prokaryotes, but ultimately eukaryotic cells including human cells). Other application themes include the development of a comprehensive simulation and informatics capability for modeling the biochemical processes of biological molecules, advanced nuclear systems, and the development of simulations of the structure and behavior of materials nanostructures. In each of these areas we seek novel proposals addressing scalable algorithms and architectures for sustaining petaflops level performance.

Rare Isotope Accelerator (RIA) (Initiative leader: Dale Knutson, OTD)
The Rare Isotope Accelerator (RIA) is an unparalleled research facility for exploring the properties of short-lived atomic nuclei near their limits of stability, as protons or neutrons are added to familiar stable nuclei. Research at the facility will illuminate the fundamental processes of the universe, such as creation of the heavier elements from which we and our world are made. Beyond contributions to the basic science of astrophysics and nuclear physics, RIA will produce unstable ("rare") isotopes having valuable technological applications. RIA has been identified by the nuclear physics community as highest priority major new construction initiative in the DOE/NSF Nuclear Science Advisory Committee's 2002 Long Range Plan. The Laboratory is pursuing significant technical developments to support the development of the RIA concept. LDRD-funded activities advance a number of the crucial technologies for RIA including the development of high efficiency structures for the acceleration of ions with very low charge to mass ratios, the beam dynamics of the entire accelerator system, high-power liquid lithium windowless fragmentation targets and thin-film stripper systems, and accelerator diagnostics for very low intensity beams. Proposals supporting the highest technical priorities for RIA are appropriate under this initiative.

Functional Genomics (Initiative leader: Lee Makowski, BIO)
In order to translate the information generated in the genome projects into a comprehensive understanding of living systems (i.e., bring the genome to life), strategies for completely characterizing the function of each protein in a cell must be developed and used. This problem constitutes one of the greatest challenges being faced by post-genome biology. Only when the functions of most, if not all, gene products are characterized will it be possible to successfully model in a predictive fashion, the responses of a cell to stimuli. We are taking a broadly interdisciplinary approach to developing tools for complete functional characterization of genomes. This approach combines informatics with high throughput experimental studies for proposing, testing and validating the functional contributions of proteins to cellular activities. The goal of this initiative is the establishment and use of a set of tools capable of quickly translating the information contained in the sequence of a genome into a comprehensive understanding of the molecular systems of the corresponding organism. The informatics efforts include novel approaches to using structure templates as a guide to function prediction based on protein sequence. The experimental efforts include high throughput cloning, expression and purification of proteins; structural genomics; protein-protein interaction mapping; proteomics; and single molecule approaches to probing function.

FY 2004 Emerging Initiative Areas

National Security Research (Initiative Leader: Starnes E. Walker, III, EEST)
Argonne proposes to expand its research, development, and analysis activities in the area of critical infrastructure assurance and counterterrorism. The goal of this work for DOE and other federal agencies is to develop and apply innovative technologies, methodologies, models and simulations that (1) will better protect critical U.S. infrastructure and associated populations from disruption; and (2) where disruptions do

occur, will improve capabilities for detection, mitigation of effects, consequence assessment, response, and recovery. The Laboratory's capabilities are particularly relevant to energy/utility infrastructures (e.g., electricity, oil, natural gas, drinking water; and their cyber-based control systems), agriculture and food supply, chemical/biological/nuclear threats, national security, transportation systems, information and communication systems, emergency services, nuclear materials and explosion monitoring, and nonproliferation technologies.

Transportation Technology (Initiative Leader: Larry Johnson, EEST)
The Transportation Technology Initiative is focused on developing advanced automotive technologies that would ultimately meet the goals of the FreedomCar and Fuel Initiative and the 21st Century Truck Partnership. The key technology for the FreedomCAR and Fuel Initiative is hydrogen-fueled fuel cells, although interim technologies that facilitate achieving the ultimate goal are needed. Key enabling technologies include: hydrogen storage, hydrogen refueling and infrastructure, fuel cell fuel processing, hybridization (including the use of hydrogen in an internal combustion engine), energy storage, and lightweight materials. In addition, advanced engine and other propulsion technologies that can significantly improve fuel economy while meeting emission standards are needed in the transition to fuel cells. Heavy truck technologies are primarily focused on dramatic reductions in diesel emissions while maintaining or even improving fuel economy. Alternative approaches to auxiliary power units (for instance, fuel cells) are also candidate technologies. Sensors, advanced instrumentation, and computational tools will be needed for advanced propulsion systems for both automobiles and trucks.

Environmental Science (Initiative leader: Chris Reilly, ER)
Several nationally identified "Grand Challenges for Environmental Science" can be approached effectively by using Argonne's unique facilities and expertise. This initiative will nucleate multidisciplinary teams to explore grand-challenge areas of environmental science that are particularly well matched to Argonne's capabilities. Two such areas, biogeochemical cycling and atmospheric particulates and aerosols, are logical first targets. (1) In biogeochemistry, the challenge is to understand how Earth's major biogeochemical cycles are perturbed by human activities; to predict the impact of these perturbations on local, regional, and global scales; and to determine how the cycles could be restored to more natural states. (2) Research on atmospheric particulates and aerosols can determine how atmospheric particles are formed, their roles in global and regional climate systems, and their relevance to chronic and acute respiratory diseases. Materials science, chemical, and physical approaches are particularly appropriate.

Hydrogen Research and Development (Initiative Leader: James F. Miller, CMT)
Secretary of Energy Spencer Abraham challenged ANL to mobilize its skills and talents to devise energy solutions for our nation's future. In the State of the Union address, President Bush announced his groundbreaking plan to transform our energy future from one dependent on foreign petroleum to one that utilizes the most abundant element in the universe – hydrogen. Hydrogen can be produced from diverse domestic sources, freeing the nation from a reliance on foreign imports. "We believe that the hydrogen economy is our future. The questions we face are how fast this effort should proceed,

and whether it will be led by America or by others." Secretary Abraham said, "The President's answer is clear: He wants this to happen in our lifetime – sooner rather than later. And he believes that the United States should lead the way. That's why the President is proposing to significantly increase our hydrogen and fuel cell spending to $1.7 billion over the next five years." Argonne will expand its research and analysis of the technologies and economics required to achieve a hydrogen economy. This will include projects on hydrogen production, co-generation, storage, transportation, distribution, safety, and economics.